



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:36 AM UTC

PDB ID : 5MU3 / pdb_00005mu3
Title : Crystal structure of Ctf19-Mcm21 kinetochore assembly bound with Ctf19-Mcm21 binding motif of central kinetochore subunit Okp1
Authors : Schmitzberger, F.
Deposited on : 2017-01-12
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

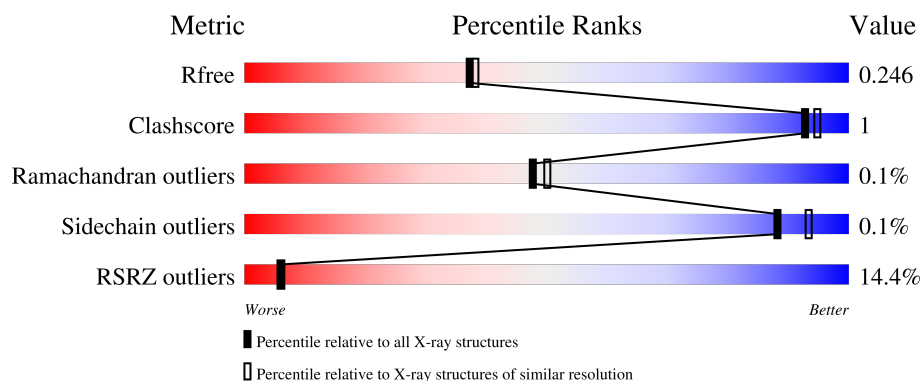
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

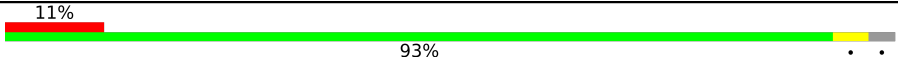
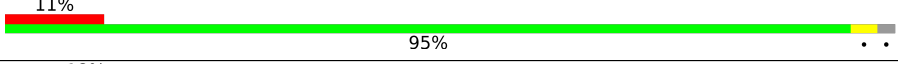
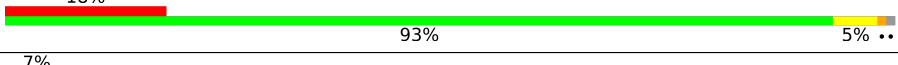
The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	189	
1	D	189	
2	B	165	
3	C	67	
3	F	67	

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Mol	Chain	Length	Quality of chain
4	E	165	16% 95%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12650 atoms, of which 6186 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Central kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	184	Total	C	H	N	O	S	0	1	0
			3046	987	1521	255	278	5			
1	D	185	Total	C	H	N	O	S	0	1	0
			3064	993	1531	256	279	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP Q6CVQ9
A	-2	ASN	-	expression tag	UNP Q6CVQ9
A	-1	ALA	-	expression tag	UNP Q6CVQ9
D	-3	SER	-	expression tag	UNP Q6CVQ9
D	-2	ASN	-	expression tag	UNP Q6CVQ9
D	-1	ALA	-	expression tag	UNP Q6CVQ9

- Molecule 2 is a protein called Central kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	163	Total	C	H	N	O	S	0	1	0
			2678	851	1354	217	249	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MET	-	initiating methionine	UNP Q6CRN7

- Molecule 3 is a protein called Central kinetochore subunit Okp1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	24	Total	C	H	N	O		0	0	0
			414	134	209	32	39				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	25	Total	C	H	N	O	0	0	0
			426	137	215	33	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	294	MET	-	initiating methionine	UNP Q6CJY0
F	294	MET	-	initiating methionine	UNP Q6CJY0

- Molecule 4 is a protein called Central kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	164	Total	C	H	N	O	S	0	0
			2684	853	1356	217	250	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	106	MET	-	initiating methionine	UNP Q6CRN7

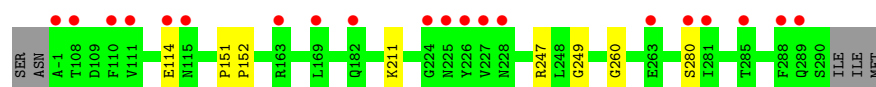
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	67	Total	O	0	0
			67	67		
5	C	20	Total	O	0	0
			20	20		
5	D	67	Total	O	0	0
			67	67		
5	E	60	Total	O	0	0
			60	60		
5	F	14	Total	O	0	0
			14	14		

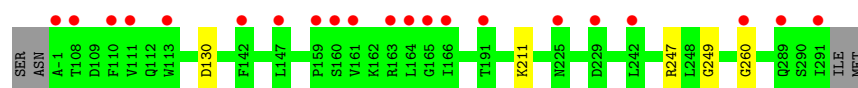
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

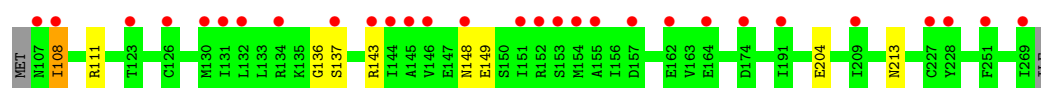
- Molecule 1: Central kinetochore subunit MCM21



- Molecule 1: Central kinetochore subunit MCM21



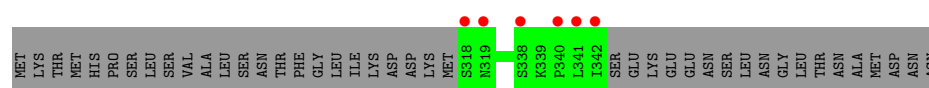
- Molecule 2: Central kinetochore subunit CTF19



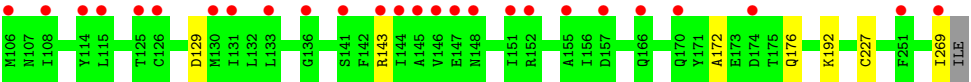
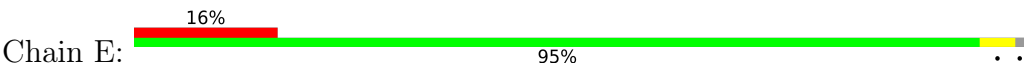
- Molecule 3: Central kinetochore subunit Okp1



- Molecule 3: Central kinetochore subunit Okp1



- Molecule 4: Central kinetochore subunit CTF19



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	93.34Å 105.48Å 122.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.06 – 2.10 80.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (80.06-2.10) 99.6 (80.06-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.222 , 0.248 0.220 , 0.246	Depositor DCC
R_{free} test set	1896 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12650	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/1564	0.25	0/2113
1	D	0.10	0/1572	0.26	0/2124
2	B	0.11	0/1349	0.28	0/1827
3	C	0.08	0/208	0.22	0/278
3	F	0.09	0/214	0.26	0/286
4	E	0.10	0/1341	0.25	0/1813
All	All	0.10	0/6248	0.26	0/8441

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1525	1521	1520	6	1
1	D	1533	1531	1531	2	1
2	B	1324	1354	1352	7	1
3	C	205	209	209	1	0
3	F	211	215	214	0	0
4	E	1328	1356	1356	5	1
5	A	110	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	67	0	0	2	0
5	C	20	0	0	0	0
5	D	67	0	0	0	0
5	E	60	0	0	1	0
5	F	14	0	0	0	0
All	All	6464	6186	6182	18	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:129:ASP:OD1	4:E:143:ARG:NH1	2.18	0.76
4:E:192:LYS:NZ	4:E:227:CSX:SG	2.60	0.74
2:B:204:GLU:OE1	5:B:301:HOH:O	2.08	0.72
1:D:247[A]:ARG:NH1	1:D:249:GLY:O	2.26	0.68
2:B:213:ASN:ND2	5:B:302:HOH:O	2.26	0.67
1:D:211:LYS:NZ	1:D:260:GLY:O	2.27	0.67
2:B:136:GLY:O	2:B:137:SER:OG	2.10	0.63
1:A:247[B]:ARG:NH1	1:A:249:GLY:O	2.38	0.54
4:E:192:LYS:NZ	4:E:227:CSX:HG	2.05	0.53
1:A:114:GLU:OE1	2:B:111:ARG:NH2	2.49	0.46
1:A:211:LYS:NZ	1:A:260:GLY:O	2.50	0.45
4:E:172:ALA:O	4:E:176:GLN:N	2.50	0.44
1:A:114:GLU:OE2	2:B:111:ARG:NH2	2.51	0.43
1:A:114:GLU:CD	2:B:111:ARG:HH21	2.27	0.42
3:C:336:ASP:OD2	3:C:339:LYS:NZ	2.43	0.42
4:E:269:ILE:O	5:E:301:HOH:O	2.22	0.41
2:B:148:ASN:OD1	2:B:149:GLU:N	2.54	0.40
1:A:151:PRO:HA	1:A:152:PRO:HD3	1.97	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ARG:NH1	4:E:129:ASP:OD1[1_565]	2.04	0.16
1:A:280:SER:OG	1:D:130:ASP:OD2[3_755]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/189 (97%)	180 (98%)	3 (2%)	0	100	100
1	D	184/189 (97%)	179 (97%)	5 (3%)	0	100	100
2	B	162/165 (98%)	153 (94%)	8 (5%)	1 (1%)	21	18
3	C	22/67 (33%)	22 (100%)	0	0	100	100
3	F	23/67 (34%)	23 (100%)	0	0	100	100
4	E	161/165 (98%)	152 (94%)	9 (6%)	0	100	100
All	All	735/842 (87%)	709 (96%)	25 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	108	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/176 (98%)	172 (100%)	0	100	100
1	D	173/176 (98%)	173 (100%)	0	100	100
2	B	151/152 (99%)	150 (99%)	1 (1%)	76	83
3	C	24/63 (38%)	24 (100%)	0	100	100
3	F	25/63 (40%)	25 (100%)	0	100	100
4	E	150/151 (99%)	150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	695/781 (89%)	694 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	108	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	170	GLN
2	B	179	ASN
1	D	128	ASN
1	D	181	HIS
4	E	110	GLN
4	E	166	GLN
4	E	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CSX	E	227	4	3,6,7	1.03	0	1,6,8	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CSX	E	227	4	-	1/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	227	CSX	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	227	CSX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	184/189 (97%)	0.71	20 (10%)	10 11	32, 56, 95, 116	1 (0%)
1	D	185/189 (97%)	0.97	21 (11%)	10 10	32, 64, 104, 125	1 (0%)
2	B	163/165 (98%)	0.94	29 (17%)	4 4	41, 60, 107, 130	1 (0%)
3	C	24/67 (35%)	1.28	5 (20%)	2 2	41, 60, 90, 118	0
3	F	25/67 (37%)	1.19	6 (24%)	2 2	45, 61, 100, 112	0
4	E	163/165 (98%)	0.88	26 (15%)	5 5	41, 61, 116, 129	0
All	All	744/842 (88%)	0.90	107 (14%)	6 6	32, 61, 107, 130	3 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	342	ILE	10.6
1	D	-1	ALA	5.9
1	A	-1	ALA	5.4
3	C	340	PRO	5.0
3	F	342	ILE	4.9
1	D	108	THR	4.7
2	B	108	ILE	4.5
2	B	146	VAL	4.3
3	F	338	SER	4.3
2	B	251	PHE	4.2
2	B	107	ASN	4.2
1	D	291	ILE	4.0
1	D	111	VAL	4.0
1	A	227	VAL	3.8
1	D	161	VAL	3.8
3	C	338	SER	3.8
1	D	164	LEU	3.8
4	E	125	THR	3.7
4	E	108	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	143	ARG	3.7
3	C	341	LEU	3.6
1	D	165	GLY	3.6
4	E	251	PHE	3.6
1	D	242	LEU	3.6
1	D	163	ARG	3.5
2	B	155	ALA	3.4
4	E	145	ALA	3.4
4	E	126	CYS	3.4
1	A	289	GLN	3.4
4	E	143	ARG	3.3
1	A	228	ASN	3.2
1	A	226	TYR	3.2
1	A	224	GLY	3.2
4	E	151	ILE	3.1
3	F	340	PRO	3.1
2	B	145	ALA	3.1
1	A	108	THR	3.0
2	B	154	MET	3.0
1	D	166	ILE	3.0
2	B	228	TYR	3.0
4	E	146	VAL	3.0
1	D	191	THR	2.9
2	B	269	ILE	2.9
3	F	319	ASN	2.9
2	B	191	ILE	2.8
2	B	144	ILE	2.8
1	A	182	GLN	2.7
2	B	148	ASN	2.7
2	B	137	SER	2.7
2	B	153	SER	2.7
2	B	164	GLU	2.6
3	F	341	LEU	2.6
4	E	147	GLU	2.6
4	E	155	ALA	2.6
1	D	160	SER	2.5
3	C	339	LYS	2.5
4	E	174	ASP	2.5
4	E	157	ASP	2.4
2	B	157	ASP	2.4
2	B	126	CYS	2.4
4	E	114	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	174	ASP	2.4
2	B	151	ILE	2.4
1	A	280	SER	2.4
2	B	162	GLU	2.3
1	A	115	ASN	2.3
2	B	130	MET	2.3
4	E	106	MET	2.3
4	E	131	ILE	2.3
1	D	260	GLY	2.3
4	E	269	ILE	2.3
1	A	163	ARG	2.3
2	B	132	LEU	2.3
2	B	152	ARG	2.3
4	E	152	ARG	2.3
4	E	166	GLN	2.3
1	D	159	PRO	2.3
2	B	227	CYS	2.3
1	A	169	LEU	2.3
1	D	113	TRP	2.3
1	A	288	PHE	2.2
1	A	111	VAL	2.2
4	E	148	ASN	2.2
1	A	285	THR	2.2
1	D	225	ASN	2.2
4	E	130	MET	2.2
4	E	133	LEU	2.2
3	F	318	SER	2.2
1	A	281	ILE	2.2
1	D	110	PHE	2.2
2	B	123	THR	2.2
1	D	142	PHE	2.1
4	E	141	SER	2.1
2	B	134	ARG	2.1
1	D	289	GLN	2.1
1	A	114	GLU	2.1
1	A	263	GLU	2.1
1	A	225	ASN	2.1
1	D	229	ASP	2.1
2	B	131	ILE	2.1
2	B	209	ILE	2.1
4	E	144	ILE	2.1
4	E	170	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	110	PHE	2.0
1	D	147	LEU	2.0
4	E	115	LEU	2.0
4	E	136	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CSX	E	227	7/8	0.88	0.14	40,54,85,102	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.